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NEWS 4 JUL 02 CHEMCATS accession numbers revised
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         JUL 18 CA/CAplus patent coverage enhanced
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NEWS 8
         JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
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         AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
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                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
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                 spectral property data
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                 STN AnaVist, Version 2.0, now available with Derwent
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         SEP 17 Caplus coverage extended to include traditional medicine
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         SEP 24
NEWS 23
         OCT 02
                CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS 24 OCT 19 BEILSTEIN updated with new compounds
NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
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              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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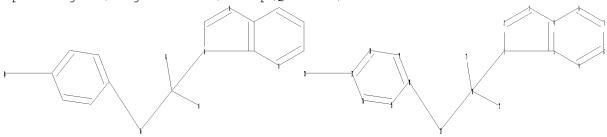
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chain nodes :

10 12 13 20 21

ring nodes :

1 2 3 4 5 6 7 8 9 14 15 16 17 18 19

chain bonds :

1-10 10-13 10-12 10-21 14-21 17-20

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 14-19 14-15 15-16 16-17 17-18 18-19

exact/norm bonds :

1-2 1-5 1-10 2-3 3-4 17-20

exact bonds :

10-13 10-12 10-21 14-21

normalized bonds :

4-5 4-6 5-9 6-7 7-8 8-9 14-19 14-15 15-16 16-17 17-18 18-19

isolated ring systems : containing 1 : 14 :

Match level:

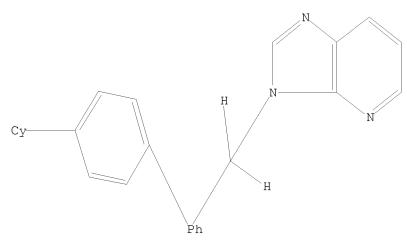
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS

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SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 06:04:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

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FULL ESTIMATED COST ENTRY SESSION 172.10 172.31

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NEWS 3 JAN 16 CAS patent coverage enhanced to include exemplified prophetic substances

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NEWS 10 FEB 20 PCI now available as a replacement to DPCI

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NEWS 12 FEB 25 IMSPRODUCT reloaded with enhancements

NEWS 13 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats

NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental spectra

NEWS 16 MAR 31 CA/Caplus and CASREACT patent number format for U.S. applications updated

NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI

NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements

NEWS 19 APR 04 STN AnaVist, Version 1, to be discontinued

NEWS 20 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
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FULL ESTIMATED COST

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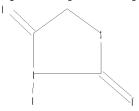
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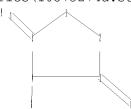
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chain nodes:
6 7 8 9
ring nodes:
1 2 3 4 5
chain bonds:
3-6 4-8 5-7

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5

exact bonds :

4-8 5-7

Match level:

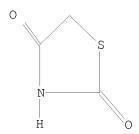
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

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L1 HAS NO ANSWERS

L1 STR



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=> s 11

SAMPLE SEARCH INITIATED 10:02:04 FILE 'REGISTRY'

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100.0% PROCESSED 380 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 6431 TO 8769

PROJECTED ANSWERS: 0 TO

L2 0 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 10:02:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7275 TO ITERATE

100.0% PROCESSED 7275 ITERATIONS 10 ANSWERS

SEARCH TIME: 00.00.01

L3 10 SEA SSS FUL L1

=> file caplus

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FULL ESTIMATED COST ENTRY SESSION 178.36 178.57

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=> s 13 full L4 5 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:445135 CAPLUS

DOCUMENT NUMBER: 141:140629

TITLE: Novel routes for the generation of structurally

diverse labdane diterpenes from andrographolide

AUTHOR(S): Nanduri, Srinivas; Nyavanandi, Vijay Kumar;

Thunuguntla, Siva Sanjeeva Rao; Velisoju, Mahendar; Kasu, Sridevi; Rajagopal, Sriram; Kumar, R. Ajaya;

Rajagopalan, R.; Iqbal, Javed

CORPORATE SOURCE: Discovery Chemistry, Discovery Research, Dr. Reddy's

Laboratories Ltd., Miyapur, Hyderabad, 500 049, India

SOURCE: Tetrahedron Letters (2004), 45(25), 4883-4886

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:140629

GΙ

AB Andrographolide, the major constituent of the Indian medicinal plant Andrographis paniculata (Acanthaceae) was converted into the key intermediate I by selective oxidative degradation of the C-12,13 olefin bond. The aldehyde functional group present in I has been utilized for synthesizing a number of structurally diverse labdane diterpenes. Synthesis and in vitro cytotoxic activity results of the compds. prepared are discussed.

IT 727723-08-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and anticancer activity of labdane diterpenes)

RN 727723-08-2 CAPLUS

CN 2,5-Thiazolidinedione, 4-[2-[(1R,4aS,5R,6R,8aS)-decahydro-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylene-1-naphthalenyl]ethylidene]-, (4E)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT:

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:322523 CAPLUS

DOCUMENT NUMBER: 125:58379

TITLE: Gas-phase elimination reactions of 4-substituted

2-alkoxythiazoline-5-ones

AUTHOR(S): Al-Awadi, Nouria; Elnagdi, Mohamed H.

CORPORATE SOURCE: Chem. Dep., Kuwait Univ., Safat, 13060, Kuwait SOURCE: Heteroatom Chemistry (1996), 7(3), 183-186

CODEN: HETCE8; ISSN: 1042-7163

PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

GΙ

AB Gas-phase elimination of 4-substituted 2-alkoxythiazoline-5-ones I (R = H, Me, X = PhNHN, 2-furylmethylene) have been studied. These compds. eliminate via a six-membered transition state to produce 4-substituted thiazolidine-2,5-diones II. These eliminations are unimol. first-order reactions. Utilization of this thermolysis reaction in the synthesis of new 4-substituted thiazolidine-2,5-diones is considered. Addnl. mechanistic information was obtained by comparing the kinetic data for thermal elimination reactions of these compds. with that of 1-ethoxythiazole.

IT 178321-12-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (kinetics of elimination of alkoxythiazolinones to thiazolidinediones)

RN 178321-12-5 CAPLUS

CN 2,5-Thiazolidinedione, 4-(2-furanylmethylene)- (CA INDEX NAME)

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:558118 CAPLUS

DOCUMENT NUMBER: 121:158118

TITLE: The synthesis of  $\beta$ -heteroarylamino- $\alpha$ ,  $\beta$ -

dehydro- $\alpha$ -amino acid derivatives via thiazolones AUTHOR(S): Smodis, Janez; Stanovnik, Branko; Tisler, Miha CORPORATE SOURCE: Dep. Chem., Univ. Ljubljana, Ljubljana, 61000,

Slovenia

SOURCE: Journal of Heterocyclic Chemistry (1994), 31(1),

199-203

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:158118

GΙ

O S OR N Me 
$$NC = C$$
 NHCOR HetNHCH I S II

AB 2-Alkoxy-4-heteroarylaminomethylene-5(4H)-thiazolones I (Het =

4,6-dimethyl-2-pyrimidyl; R = Me, Ch2Ph, Et; Het = 4-methyl-2-pyrimidyl, R

= Me) were converted with various nucleophiles into  $\beta$ -heteroarylamino-

 $\alpha$ ,  $\beta$ -dehydro  $\alpha$ -amino acid derivs. II (R = Me, CH2Ph), III

(Het = 4,6-dimethyl-2-pyrimidyl; R = Me, Ch2Ph, Et, R1 = OMe; Het =

4-methyl-2-pyrimidyl, R = Me, R1 = OMe; Het = 4,6-dimethyl-2-pyrimidyl; R

= Me, Ch2Ph, R1 = NH2; Het = 4-methyl-2-pyrimidyl, R = Me, R1 = NH2; Het =

4,6-dimethyl-2-pyrimidyl, R = Me, R1 = NMe2; Het = 4,6-dimethyl-2-

pyrimidyl, R = CH2Ph; R1 = NHNH2), and peptide derivative III (Het =

4,6-dimethyl-2-pyrimidyl; R = Me, R1 = NHCH2CO2H). Reduction of I with sodium borohydride in EtOH saturated with gaseous ammonia afforded the corresponding  $\beta$ -heteroarylamino substituted alanyl amides

HetNHCH2CH(CONH2)NHC(S)OR. Thiazoledione derivative IV was transformed with sodium methoxide in methanol into imidazol-2(3H)-one V.

IT 157423-82-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and rearrangement of, to imidazole derivative)

RN 157423-82-0 CAPLUS

CN 2,5-Thiazolidinedione, 4-[[(4,6-dimethyl-2-pyrimidinyl)amino]methylene]- (CA INDEX NAME)

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1961:137436 CAPLUS

DOCUMENT NUMBER: 55:137436

ORIGINAL REFERENCE NO.: 55:25919g-i,25920a-h

TITLE: Action of Grignard reagents. XXII. Action of

organo-magnesium compounds on 2-thioxo-4-arylidene-5-

thiazolidones and on 4-arylidene-2,5-

thiazolidinediones. Reaction of 2-thioxo-4-benzylidene-

5-thiazolidone with diazomethane

AUTHOR(S): Mustafa, Ahmed; Sallam, Mohamed Mohamed

CORPORATE SOURCE: Cairo Univ., Giza, Egypt

SOURCE: Journal of Organic Chemistry (1961), 26, 1782-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AΒ Treatment of 2-thioxo-4-arylidene-5-thiazolidones with organomagnesium compds. did not effect the opening of the heterocyclic N ring, but only addition to the conjugation created by attachment of an exocyclic double bond in the 4-position took place to give colorless products, believed to have the general structure ArCHRCH.CO.S.CS.NH. 2-Thioxo-4-diphenylmethyl-5thiazolidone (I) was also obtained by the addition of C6H6 to the exocyclic double bond in 2-thioxo-4-benzylidene-5-thiazolidone (II) in the presence of anhydrous AlCl3. Hydrolysis of the Grignard products, ArCHRCH.CO.S.CS.NH, exemplified by I and PhCHEtCH.CO.S.CS.NH (III), with aqueous 10% NaOH established a new route for the preparation of  $\beta$ ,  $\beta$ -disubstituted alanines, namely,  $\beta,\beta\text{-diphenyl-}$  (IV) and  $\beta\text{-phenyl-}\beta\text{-}$ ethylalanine (V). Similarly, addition of organomagnesium compds. to the exocyclic double bond in the newly prepared 4-arylidene-2,5thiazolidinediones took place with formation of colorless products, believed to have structures ArRCHCH.CO.S.CO.NH. Hydrolysis of  $4-(\alpha-phenylpropy1)-2$ , 5-thiazolidinedione (VI) with aqueous NaOH gave IV. The action of ethereal CH2N2 on II led to the formation of 2-methylthio-4-benzylidene-5-thiazolidone (VII) in good yield. Na (4.9 g.) in 120 ml. alc. added during 2 hrs. to 26 g. aminoacetonitrile sulfate in 150 ml. Me2CO, 17 ml. CS2 and then 200 ml. Et2O added to the filtrate, the 18 g. of solid obtained dissolved in H2O, and this solution added to 300 ml. Me2CO gave 14.4 g. carbamoylmethylammonium carbamoyldithiocarbamate (VIII), m. 138-9° (decomposition). VIII (1 g.) in 6 ml. H2O treated with 0.5 q. p-tolualdehyde in 3 ml. alc. and the mixture treated dropwise with 3 ml. HCl gave 0.15 g. 2-thioxo-4-(p-methylbenzylidene)-5thiazolidone, yellow needles, m. 220-1° (C6H6). A Grignard solution (from 0.9 g. Mg and 9 g. PhBr in 50 ml. Et20) added to 1.5 g. of each member of a series of 2-thioxo-4-arylidene-5-thiazolidones (arylidene group = PhCH:, p-MeOC6H4CH:, p-MeC6H4CH:, : CHC6H3O2CH2-3,4) in 50 ml. C6H6, the Et2O evaporated, the mixture heated 1 hr., kept 3 hrs. at room temperature,

poured onto 100 ml. saturated NH4Cl containing 3 ml. HCl, extracted with C6H6, and the  $\,$ 

solvent evaporated gave solid residues, which were crystallized The Grignard products, ArCHRCH.CO.S.CS.NH, were similarly prepared, colorless, soluble in cold 10% NaOH, no color with alc. FeCl3, generally soluble in hot C6H6, and difficultly soluble in ligroine (Ar and R or compound number, solvent of crystallization,

m.p., % yield, and color with H2SO4 given): I, alc., 199-200°, 76, yellow; Ph, p-tolyl, alc., 173°, 88, yellow; Ph, Me, C6H6, 170°, 82, no color; III, C6H6-ligroine, 157-8°, 79, no color; Ph, iso-Pr, C6H6, 214°, 76, no color; p-MeOC6H4, Ph, alc., 139°, 74, yellow; p-MeOC6H4, p-tolyl, C6H6, 149°, 70, orange; p-MeOC6H4, Me, C6H6-ligroine, 175°, 72, no color; p-MeOC6H4, Et, C6H6, 167°, 78, no color; p-MeOC6H4, Ph, alc., 173°, 68, yellow; C6H3O2-CH2-3,4, Ph, C6H6, 212°, 71, red;

C6H302CH2-3,4, p-tolyl, C6H6, 195°, 73, red; C6H302CH2-3,4, Me, C6H6, 184°, 72, yellow. I (1 g.) and 10 ml. aqueous NaOH refluxed 15 min., the mixture cooled, poured on ice, and acidified gave 0.55 g. IV, m. 234-5° (decomposition); HCl salt m. 227° (decomposition). IV (0.5 g.) in 5 ml. aqueous 10% NaOH treated 15 min. with 0.4 ml. BzCl, poured on ice, acidified, the solid triturated with 3 ml. hot CCl4, and crystallized gave 0.35 g. Bz derivative (IX), m. 190-1° (dilute alc.). IX (0.5 g.) and 0.3 g. fused NaOAc heated 0.5 hr. with 0.5 ml. Ac2O gave 0.15 g. 2-phenyl-4-diphenylmethyl-5(4H)-oxazolone, m. 158° (C6H6-ligroine). III (1 g.) similarly treated with NaOH gave 0.6 g. V, m. 222-3° (decomposition). Benzoylation of V gave 0.3 g. Bz derivative, m. 193°. II (6 g.) in 200 ml. C6H6 added at 10-20° to 9.5 g. AlCl3 and 125 ml. C6H6, the mixture stirred 3 hrs. at room temperature, the complex decomposed

dilute HCl, extracted with C6H6, and crystallized gave 4.1 g. I. 2,5—Thiazolidinedione (5 g.), 5 ml. BzH, and 20 ml. AcOH refluxed 0.5 hr. with 3 g. fused NaOAc gave 3.2 g. 4-benzylidene-2,5-thiazolidinedione (X), m. 165° (alc.). Similarly, refluxing 5 g. 2,5-thiazolidinedione, 5 ml. p-methoxybenzaldehyde, 20 ml. AcOH, and 3 g. fused NaOAc 0.5 hr. gave 2.9 g. 4-(p-methoxybenzylidene)-2,5-thiazolidinedione (XI), m. 168° (alc.). Grignard reagents treated with X and XI gave VI and related compds. The following results were obtained (starting material, Grignard product Ar and R or compound number, solvent, m.p., % yield, and color with H2SO4 given): X, VI, C6H6, 136°, 82, yellow; X, Ph, p-MeOC6H4, alc., 145°, 70, orange; X, Ph, Me, alc., 159°, 81, no color; XI, p-MeOC6H4, Me, alc., 149°, 73, no color. VI (1 g.) in 10 ml. 10% NaOH gave 0.45 g. IV. II (1 g.) in 50 ml. Et2O kept overnight at 0° with CH2N2 gave 0.8 g. VII, m. 101° (ligroine).

IT 103038-18-2P, 2,5-Thiazolidinedione, 4-benzylidene-103853-89-0P, 2,5-Thiazolidinedione, 4-p-methoxybenzylidene-RL: PREP (Preparation)

(preparation of) RN 103038-18-2 CAPLUS

CN 2,5-Thiazolidinedione, 4-benzylidene- (6CI) (CA INDEX NAME)

with

RN 103853-89-0 CAPLUS

CN 2,5-Thiazolidinedione, 4-p-methoxybenzylidene- (6CI) (CA INDEX NAME)

L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1952:14468 CAPLUS

DOCUMENT NUMBER: 46:14468
ORIGINAL REFERENCE NO.: 46:2524e-h

TITLE: 2,5-Thiazolidinedione

AUTHOR(S): Aubert, Per; Jeffreys, R. A.; Knott, E. B.

CORPORATE SOURCE: Kodak Ltd., Wealdstone, UK

SOURCE: Journal of the Chemical Society (1951) 2195-7

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 46:14468
GI For diagram(s), see printed CA Issue.

For diagram(s), see printed CA Issue. HO2CCH2NHCSOEt (5 g.) in 15 cc. C6H6, treated with PCl3 and gently warmed to about 40°, gives 75% 2,5-thiazolidinedione (I), m. 110°; the yield is the same with 2.2 or 0.33 mol. PCl3 or with PBr3; the yields are lower in C6H6-dioxane. CO.CH2.N:C(OEt).S (5 g.) in 15 cc. C6H6, treated with 3 cc. PBr3, gives 2.9 g. I. 2,2'-Acetanilidovinylbenzoxazole-EtI (2.2 g.) in 150 cc. EtOH, treated at 30° with 0.5 cc. Et3N and 0.6 g. I, and kept 2 days, gives [2-(3-ethylbenzoxazole)][4-(2,5thiazolidinedione)]dimethinemerocyanine (II), orange, m. 248°; if the components in 10 cc. EtOH are boiled 15 min., the yellow solution becomes deep crimson and gives a sepia dye, m.  $257^{\circ}$ , which is II plus 1 mol. EtOH. I (1 g.) in 15 cc. H2O, heated 1 min. on the steam bath, give a polyglycine, amorphous, darkens about 300°. MeCH(NH2)CO2H (20.8 g.) and 12.1 g. KOH in 40 cc. H2O, treated with 35 g. EtOCS2Et in 40 cc. EtOH and heated 24 hrs. on the steam bath, give 21 g. N-thionocarbethoxy-DL-alanine, m.  $103.5^{\circ}$ ; sarcosine (5 g.) gives 9.5 g. N-thionocarbethoxysarcosine, m. 86°; these compds. on

cyclodealkylation give oils.
IT 854163-58-9P, 2,5-Thiazolidinedione, 4-[2-(3-ethyl-2-benzoxazolinylidene)ethylidene]- 854163-59-0P, Benzoxazole,
2-[2-(2,5-dioxo-4-thiazolidinylidene)ethylidene]-3-ethyl-, compound with EtOH

RL: PREP (Preparation) (preparation of) 854163-58-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 854163-59-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

RN

CRN 854163-58-9 CMF C14 H12 N2 O3 S

CM 2

CRN 64-17-5 CMF C2 H6 O

н<sub>3</sub>С-Сн<sub>2</sub>-Он

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(FILE 'HOME' ENTERED AT 10:01:34 ON 17 APR 2008)

FILE 'REGISTRY' ENTERED AT 10:01:42 ON 17 APR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

CA SUBSCRIBER PRICE

L3 10 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:02:13 ON 17 APR 2008

L4 5 S L3 FULL

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COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
28.69 207.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

-4.00

-4.00

STN INTERNATIONAL LOGOFF AT 10:04:01 ON 17 APR 2008